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Classification of the Super-conducting order parameters under the point group symmetry for a multi-band system: application to LaOFeAs

Zhi-Hui Wang[1], Hui Tang[2,1], Zhong Fang[2] and Xi Dai[2]

[1]*Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, China and*

[2]*Beijing National Laboratory for Condensed Matter Physics,*

*and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China**

Abstract

All the possible super-conducting order parameters for the LaOFeAs system are classified by their transformation under the complete crystal symmetry. The general forms of the super-conducting gap functions for each class are discussed. We find that the gap functions in such a multi-band system belong to three types, full gap, nodal type and finite "Fermi arc" type. Possible physical consequences caused by different types of gap functions are also discussed.

*Electronic address: daix@aphy.iphy.ac.cn

I. INTRODUCTION

The iron based superconductors, the second family of the high temperature superconducting materials, have been discovered very recently. Hosono group first obtained superconductivity in LaOFeAs with $T_c = 26K$ by replacing some Oxygen atom with F [1]. Soon after it, super-conductivity is discovered in several similar materials with T_c = 41 K in $CeO_{1-x}F_xFeAs$ [2] and $T_c = 43$ K in $SmO_{1-x}F_xFeAs$ [3]. Further replacing La atoms with other rare earth elements rapidly raises T_c up to $52K$ in $Pr[O_{1-x}F_x]FeAs$ [4] and $55K$ in $Sm[O_{1-x}F_x]FeAs$ [5]. With some other ways to introduce carriers, super-conductivity with the T_c= $55K$ in $Gd_{1-x}Th_xOFeAs$ and $ReFeAsO_{1-\delta}$ are obtained by several groups [6, 7, 8].

N. L. Wang's and Z. Fang's group first reported that the ground state of the parent compound shows SDW long range order with stripe like spin configuration by combining the first principle calculation and optical measurement [9]. The SDW state has been confirmed by neutron scattering results from two independent groups [10, 11], and several other calculations[12, 13]. The NMR data also show strong evidence of magnetic phase transition at 135K [14, 15], which is consistent with the previous neutron scattering and optical conductivity experiments. Upon F doping, the SDW is suppressed very quickly and superconductivity appears. Since the maximum T_c achieved in this family is around 55K, which is well above the McMillan limit, the super-conductivity here is likely to be non-BCS type.

The pairing symmetry of the super-conductivity in iron based super-conductors is one of the key issues. The strong magnetic fluctuation, which is suggested by the first principle calculation [9, 16, 17, 18, 19, 20, 21] and NMR measurement [14, 15], is considered by many authors to be the "pairing glue". However it is still under debate if the ferromagnetic[16, 17, 22] or anti-ferromagnetic[12, 13] fluctuation is responsible for the super-conductivity here. The ferromagnetic (anti-ferromagnetic) fluctuation will mediate attractive interaction in the spin triplet (singlet) channel and thus leads to the triplet (singlet) super-conducting state[23, 24, 25, 26, 27, 28]. The current experimental data still can not confirm the spin state of the Cooper pairs and band structure calculation indicates nearly degenerate multiple Fermi Surfaces (FS) in the system [22]. Therefore at the current stage, there still exist many possible pairing order parameters leading to many different types of gap functions . It is then important to classify all these possible super-conducting order parameters by their different transformation behavior under the full symmetry of the crystals, which will be done

in the following sections. After the classification, we will obtain many classes of the super-conducting order parameters with each of them forming an irreducible representation of the full symmetry the system have. Also we will discuss the general form of the gap functions for each class of the super-conducting phase, which can be grouped into three catalogs. The simplest type, which is referred to type (I) gap function, has a fully opened gap over the whole FS for any non-zero order parameter. The type (II) gap function contains a nodal point on the FS where it vanishes. And the type (III) gap function will vanish on a finite section of the FS, which is mentioned as "Fermi arc" in the previous literature [23].

II. CLASSIFICATION OF THE SUPER-CONDUCTING ORDER PARAMETERS

The full symmetry of the crystal can be view as the direct production of time reversal, spacial inversion, charge conservation,translational symmetry and the point group symmetry. In the present study, we assume that the appearance of super-conductivity only breaks the charge conservation and keeps all the other symmetry. The purpose of the current paper is to classify all the possible super-conducting order parameters by the group representation theory.

A. The Fermi surface topology and the point group symmetry of $LaOFeAs$

In the absence of SDW state (after F-doping), LaOFeAs crystallizes in layered square lattice with space group P4/nmm. There are two Fe sites per unit cell, which are coordinated by As-tetrahedrons. The point group symmetry of $LaOFeAs$ is D_{4h}, which contains a 4-fold rotational axis along z-direction, four vertical reflection planes along x, y, xy and $\bar{x}y$ directions, a horizontal reflection plane, as well as the spacial inversion. According to the first principle calculation, for non magnetic $LaOFeAs$, [16, 17, 18, 19, 20, 21]there are two hole type Fermi surfaces enclosing Γ point and two electron type Fermi surfaces enclosing M point. Upon F doping, the three hole type Fermi surfaces shrink rapidly and will be neglected in the present paper. Therefore we can focus on the super-conducting order parameters on the two electron type Fermi surfaces. The shape of the Fermi surfaces enclosing M point is very close to ellipse with their long axis along $(1,1)$ or $(\bar{1},1)$ directions. The first principle calculation indicates that the states around the FS around M point are mainly from the

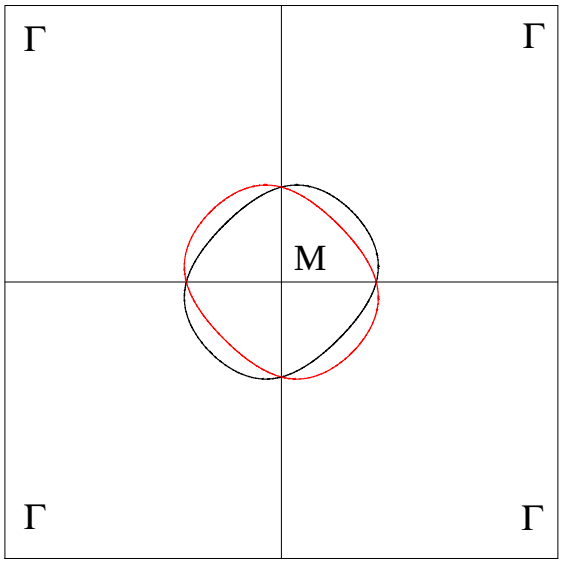

Figure 1: The schematic Fermi surface of the LaOFeAs, the FS of band 1 (2) is plotted by the black (red) ellipse.

$xy, xz$and yz iron 3d orbitals with very strong angle dependence along the FS [22]. Before we begin to classify all the possible superconducting order parameter $\Delta(\mathbf{k})$for a multi-band system, we first have to define the Bloch states $\psi_{n\boldsymbol{k}}(r)$ around M point properly to guarantee$\psi_{n\boldsymbol{k}}(r)$ to be smoothly connected along the momentum space. This "smooth condition" give us unique definition of the energy bands, which gives the ellipse FS for band "1" ("2") along $(1,1)$ ($(\bar{1},1)$)directions as shown in Fig. 1.

By definition the origin for all the point group operations and spacial inversion should be located at Γ point. While one can easily prove that using the periodicity of the momentum space, the origin can be moved to M point. Therefore in the following of the paper, all the point group and spacial inversion operations are taken respect to the M point.

With such a smooth condition for the energy bands, we can write down the effect of the D_{4h} group elements $\hat{g}_l$ acting on the Bloch functions in the two bands forming the FS around the M point. In general it can be written as

$$\hat{g}_l \psi_{n\boldsymbol{k}}(r) = \hat{D}^{orb}_{mn}(\hat{g}_l)\, \psi_{n\hat{\mathbf{D}}^{\mathbf{R}(-)}(\hat{\mathbf{g}}_\mathbf{l})\boldsymbol{k}}(r)$$

where 2×2 matrices $\hat{D}^{orb}_{mn}(\hat{g}_l)$ are the representation matrices in the orbital space, which equal to unit matrix for operators $\left(E, C_2^{"}, i, 2\sigma_v^{"}\right)$and σ_x for the rest of them. The above representation in the orbital space can be checked by the symmetry right on the FS. From

Fig.1, one can easily find that the FS of band "1" ("2") remains unchanged under the first catalog of the operators and transforms to FS of band "2" ("1") under the second catalog of the operators.

B. The super-conducting order parameter and its transformation under D_{4h}

In the multi-band system, the super-conducting order parameter can be written as

$$\Delta_{\mu\nu}^{\alpha\beta}(k) = \langle C_{\alpha\mu}(k) C_{\beta\nu}(-k) \rangle$$

where $\alpha, \beta = 1, 2$ are the band Indies, $\mu, \nu = \downarrow, \uparrow$ denote the electron spin. The functions $\Delta_{\mu\nu}^{\alpha\beta}(k)$ form a representation of the full symmetry of the system, which can be expressed as the direct production of time reversal, spacial inversion and point group symmetry. In addition, the anti-symmetric nature of the fermionic many body wave function requires $\Delta_{\mu\nu}^{\alpha\beta}(k) = -\Delta_{\nu\mu}^{\beta\alpha}(-k)$. In the present study, we follow the treatment of Sigrist and Ueda on the effect of spin-orbital coupling (SOC)[29], assuming the SOC is not too strong so that the induced coupling between the singlet and triplet pairing states can be safely neglected. Therefore we can first divide $\Delta_{\mu\nu}^{\alpha\beta}(k)$ into singlet and triplet two subgroups. Among them, the singlet pairing order parameter can be written as a 2×2 matrix $\Delta_{singlet}^{\alpha\beta}(k)$ with the following requirement from the anti-symmetric condition upon particle exchange,

$$\Delta_{singlet}^{\alpha\beta}(k) = \Delta_{singlet}^{\beta\alpha}(-k)$$

. Therefore for even (odd) parity state $\Delta_{singlet}^{\alpha\beta}(k)$ must be a symmetric (anti-symmetric) matrix. Following the standard notation the order parameters for the triplet pairing state[30] can be expressed by a vector $\overrightarrow{d}^{\alpha\beta}(k)$with each component of the d-vector to be a 2×2 matrix. And the requirement from the anti-symmetric condition here is

$$\overrightarrow{d}^{\alpha\beta}(k) = -\overrightarrow{d}^{\beta\alpha}(-k)$$

, where for even (odd) parity states $\overrightarrow{d}^{\alpha\beta}(k)$ must be anti-symmetric (symmetric) matrices. With the above notation of the super-conducting order parameters for both singlet and triplet pairing states, we can write down the symmetry transformations of these order parameters under time reversal and point group operators. For time reversal symmetry we have

$$K\Delta_{singlet}^{\alpha\beta}(k) = \Delta_{singlet}^{\alpha\beta *}(-k)$$

, for spin singlet states and

$$K\overrightarrow{d}^{\alpha\beta}(k) = -\overrightarrow{d}^{\alpha\beta *}(-k)$$

.

At last we consider the symmetry transformation under point group operators, which are group elements of D_{4h}. As we have mentioned before, in the present study, the energy scale of spin-orbital coupling is considered to be small compared with the energy splitting between the spin spin singlet and triplet pairing states but is still big enough to lift the degeneracy in the spin space spanned by vector $\overrightarrow{d}^{\alpha\beta}$. As the consequence, the spin degree of freedom of the Cooper pairs has to be frozen to the spacial motion of the electrons. Therefore the d-vector has to rotate exactly following the momentum $\boldsymbol{k}$ under the point group operators, which leads to

$$\hat{g}_l \overrightarrow{d}^{\alpha\beta}(\boldsymbol{k}) = \hat{D}^{R(+)}(\hat{g}_l)\overrightarrow{d}^{\alpha\beta}\left(\hat{D}^{R(-)}(\hat{g}_l)\boldsymbol{k}\right)$$

where $\hat{D}^{R(\pm)}$ is the representation in three-dimensional space with positive (for spin space) or negative (for k-space) spacial inversion operation respectively.

By the transformation under symmetry operators, we can construct a representation of the full crystal symmetry using the super-conducting order parameters as the basis. As we have mentioned above, the two corresponding Bloch bands we are interested in are defined smoothly in k-space. Therefore the SC order parameters $\triangle_{\mu\nu}^{\alpha\beta}(k)$ should be also smooth function in k-space, which allows us to expand them by first three sphere harmonics and use them as the basis for k dependence.

In general such a representation is reducible and can be reduced to a serial of irreducible representations. In the following two sections, we will list all the irreducible representations and discuss the corresponding basis functions for both the singlet and triplet super-conducting states in $LaOFeAs$.

Table I: Basis gap functions for the symmetry D_{4h} (a). Spin-Singlet

	$\mathcal{T}$	P	O	S	Basis	Gap type
A_{1g}	+	+	+	−	$\sigma_0(x^2+y^2),\ \sigma_1(x^2+y^2),\ \sigma_0(2z^2-x^2-y^2),\ \sigma_3(xy),\ \sigma_1(2z^2-x^2-y^2)$	I;II;III
A_{2g}	+	+	+	−	$\sigma_3(x^2-y^2)$	II
B_{1g}	+	+	+	−	$\sigma_0(x^2-y^2),\ \sigma_1(x^2-y^2)$	II;III
B_{2g}	+	+	+	−	$\sigma_3(x^2+y^2),\ \sigma_0(xy),\ \sigma_3(2z^2-x^2-y^2),\ \sigma_1(xy)$	II;III
E_g	+	+	+	−	$\sigma_0(xz),\ \sigma_0(yz),\ \sigma_3(xz),\ \sigma_3(yz),\ \sigma_1(xz),\ \sigma_1(yz)$	II,III
B_{1u}	−	−	−	−	$i\sigma_2(z)$	II,III
E_u	−	−	−	−	$i\sigma_2(y),\ i\sigma_2(x)$	II;III

C. The irreducible representation and basis gap functions for spin singlet superconducting state in $LaOFeAs$.

In the above table, we list all the basis gap functions for spin-singlet super-conducting states in $LaOFeAs$, where σ_0 , σ_1, σ_2 , σ_3 are 2×2 unit matrix and Pauli matrices respectively, which form a complete basis for the orbital space. On the first three columns we list the even-odd properties of the basis function under the time reversal (T), spacial inversion (P), spin exchange (S) and orbital exchange (O), with the plus and minus sign representing the even and odd functions under the transformation respectively. The anti-symmetric condition for the Fermion exchange requires $P\cdot S\cdot O=-1$, which is well satisfied by each basis function. Due to the multi-band nature, the system show some interesting feature which is different with the single band case. Firstly because of the additional orbital degree of freedom, it is possible to have odd parity basis functions for spin singlet phase, as in representation B_{1u} and E_u. Secondly in A_{1g} and B_{2g}, the s-wave basis functions can mix with some d-wave basis functions. This is because the special FS topology around the M point. The two electron type FS enclosing M point form a 2-dimensional representation for D_{4h}. If we only consider the pairing order parameters within one particular band, the D_{4h} symmetry will be broken.

In the following, we will discuss in deal the super-conducting gap functions for A_{1g},which is the trivial representation of D_{4h}, as an example. In this case, the super-conducting order parameter can be written as the linear combination of the three in-plane basis functions,

which reads,

$$\Delta_s^{11}(k) = a\left(cos(k_x) + cos(k_y)\right) + bsin(k_x)sin(k_y)$$

$$\Delta_s^{22}(k) = a\left(cos(k_x) + cos(k_y)\right) - bsin(k_x)sin(k_y)$$

$$\Delta_s^{12}(k) = \Delta_s^{21}(k) = c\left(cos(k_x) + cos(k_y)\right)$$

With the different value of a,b and c, the super-conducting gap may have following three different types.

1. Full energy gap, which is labeled by I in the above table. When the intra-band s-wave component $a \neq 0$, there is finite energy gap right on the Fermi level for the whole FS.

2. Energy gap with a nodal line along the x and y axises, which is labeled by II . In order to have nodal lines in this particular representation, we must have $a = c = 0$ and $b \neq 0$. In this case the super-conducting gap vanishes at four FS crossing points.

3. Fermi arc which is labeled by III. With this type of gap structure, there is a finite section of FS which remains ungaped, which is first proposed by us in reference [23] . This situation may happen when only inter-band pairing strength $c \neq 0$.

The second important representation for the singlet pairing states in $LaOFeAs$ is B_{1g} , within which the SC order parameters are linear combinations of the intra-band and inter-band $d_{x^2-y^2}$states. In this case the pairing is the strongest at four FS crossing points and vanishes along the x and y axises. When only the inter-band component is non-zero, the gap function will have a "Fermi arc".

D. The irreducible representation and basis gap functions for spin triplet super-conducting state in $LaOFeAs$.

In the above table, we list all the basis gap functions for spin-triplet super-conducting states in $LaOFeAs$. Since the total spin of the Cooper pairs generate extra degree of freedom, the situation for the spin triplet SC states is more complicated. In the present

Table II: Basis gap functions for the symmetry D_{4h} (b). Spin-Triplet

	$\mathcal{T}$	P	O	S	Basis	Gap type
A_{1g}	$-$	$+$	$-$	$+$	$i\sigma_2[\vec{e}_z(x^2-y^2)],\ i\sigma_2[\vec{e}_x(yz)+\vec{e}_y(xz)]$	III
A_{2g}	$-$	$+$	$-$	$+$	$i\sigma_2[\vec{e}_z(xy)],\ i\sigma_2[\vec{e}_x(xz)-\vec{e}_y(yz)]$	III
B_{1g}	$-$	$+$	$-$	$+$	$i\sigma_2[\vec{e}_z(x^2+y^2)],\ i\sigma_2[\vec{e}_z(2z^2-x^2-y^2)],\ i\sigma_2[\vec{e}_x(yz)-\vec{e}_y(xz)]$	I;II;III
B_{2g}	$-$	$+$	$-$	$+$	$i\sigma_2[\vec{e}_x(xz)+\vec{e}_y(yz)]$	III
E_g	$-$	$+$	$-$	$+$	$i\sigma_2[\vec{e}_x(x^2+y^2)],\ i\sigma_2[\vec{e}_y(x^2+y^2)],\ i\sigma_2[\vec{e}_x(2z^2-x^2-y^2)],\ i\sigma_2[\vec{e}_y(2z^2-x^2-y^2)]$ $i\sigma_2[\vec{e}_x(x^2-y^2)],\ i\sigma_2[\vec{e}_y(x^2-y^2)],\ i\sigma_2[\vec{e}_x(xy)],\ i\sigma_2[\vec{e}_y(xy)]$ $i\sigma_2[\vec{e}_z(xz)],\ i\sigma_2[\vec{e}_z(yz)]$	I;II;III
A_{1u}	$+$	$-$	$+$	$+$	$\sigma_0[\vec{e}_x(x)+\vec{e}_y(y)],\ \sigma_0[\vec{e}_z(z)],\ \sigma_3[\vec{e}_x(y)+\vec{e}_y(x)],\ \sigma_1[\vec{e}_x(x)+\vec{e}_y(y)],\ \sigma_1[\vec{e}_z(z)]$	I;II;III
A_{2u}	$+$	$-$	$+$	$+$	$\sigma_0[\vec{e}_x(y)-\vec{e}_y(x)],\ \sigma_3[\vec{e}_x(x)-\vec{e}_y(y)],\ \sigma_1[\vec{e}_x(y)-\vec{e}_y(x)]$	I;II;III
B_{1u}	$+$	$-$	$+$	$+$	$\sigma_0[\vec{e}_x(x)-\vec{e}_y(y)],\ \sigma_3[\vec{e}_x(y)-\vec{e}_y(x)],\ \sigma_1[\vec{e}_x(x)-\vec{e}_y(y)]$	I;II;III
B_{2u}	$+$	$-$	$+$	$+$	$\sigma_0[\vec{e}_x(y)+\vec{e}_y(x)],\ \sigma_3[\vec{e}_x(x)+\vec{e}_y(y)],\ \sigma_3[\vec{e}_z(z)],\ \sigma_1[\vec{e}_x(y)+\vec{e}_y(x)]$	I;II;III
E_u	$+$	$-$	$+$	$+$	$\sigma_0[\vec{e}_x(z)],\ \sigma_0[\vec{e}_y(z)],\ \sigma_0[\vec{e}_z(x)],\ \sigma_0[\vec{e}_z(y)],\ \sigma_3[\vec{e}_x(z)],\ \sigma_3[\vec{e}_y(z)],$ $\sigma_3[\vec{e}_z(x)],\ \sigma_3[\vec{e}_z(y)],\ \sigma_1[\vec{e}_x(z)],\ \sigma_1[\vec{e}_y(z)],\ \sigma_1[\vec{e}_z(x)],\ \sigma_1[\vec{e}_z(y)]$	I;II;III

study, we will only focus on the possible gap structure. The first five representations with even parity are purely inter-band pairing states. In the previous paper, we have discussed the gap structure of inter-band s-wave and $d_{x^2-y^2}$-wave states , which are listed in theB_{1g} and A_{1g} representations respectively. For the inter-band s-wave state with order parameter $i\sigma_2[\vec{e}_z(x^2+y^2)]$, the system will have full gap at the FS when the amplitude of the pairing order parameter is much bigger than the maximum splitting of the two bands at the FS and will have "Fermi Arc" behavior otherwise[23]. And as we have discussed in the previous paper, for the inter-band $d_{x^2-y^2}$ state, the "Fermi Arc" will always appear around the diagonal line. The basis functions in theB_{2g} and A_{2g} representations describe the inter-band pairing states along the c-axis, which are very unlikely for a layered compound like $LaOFeAs$.

The basis functions in the rest of the triplet representations mainly describe the intra-band p-wave pairing states. But they can be mixed with the corresponding inter-band p-wave pairing states. The A_{1u} representation contains three in-plane pairing states, namely $\sigma_0[\vec{e}_x(x)+\vec{e}_y(y)]$, $\sigma_3[\vec{e}_x(y)+\vec{e}_y(x)]$ and $\sigma_1[\vec{e}_x(x)+\vec{e}_y(y)]$. The first one is quite well known in the Helium III system as the BW phase. While in the present two-band system,very

interestingly the BW phase here may be mixed with two other states. The first one is an intra-band pairing state with the order parameter $\overrightarrow{d} = \sigma_3[\vec{e}_x(y) + \vec{e}_y(x)]$, and another one is an inter-band pairing state with $\overrightarrow{d} = \sigma_1[\vec{e}_x(x) + \vec{e}_y(y)]$, which is nothing but the inter-band BW phase. Although the intra-band BW phase itself has a full energy gap on the FS, it may acquire line nodes or "Fermi Arc" after mixing with the intra-band BW phase. We will discuss the physical properties of this state in detail in a separated paper. The behavior of the energy gaps for the A_{2u},B_{1u} and B_{2u} states are quite similar with that of A_{1u} states. Another important representation for the triplet states is E_u, which contains the ABM phase in Helium III system. The intra-band ABM phase, which is proposed by M. Sigrist and M. Rice for the super-conductivity in $SrRuO_4$, can be obtained by linear combination of two basis, namely $\sigma_0[\vec{e}_z(x)]$ and $\sigma_0[\vec{e}_z(y)]$. The intra-band ABM phase breaks the time reversal symmetry and also can mix with the inter-band ABM phase. Similarly for purely inter-band ABM phase, the "Fermi Arc" behavior will appear.

III. CONCLUSIONS

In the present study, we classified the possible super-conducting order parameters for $LaOFeAs$ systems respect to all the crystal symmetry including time reversal, inversion and point group symmetry. Since the spin-orbital coupling in the system is weak, we can still divide the possible super-conducting order parameters into spin singlet and triplet two classes. The for each class we give the detailed classification table with each class forming an irreducible representation. We also discussed the possible gap structure for each class of super-conducting phases. In the $LaOFeAs$ system, partly due to its multi-band nature, there are three possible types of gap functions, namely full gap, nodal gap and "Fermi Arc" type. The different types of super-conducting gap will have very different thermal dynamic and super-conducting properties in low temperature, i.e. the specific heat and superfluid density. The super-conducting state with full gap, like s-wave, will have exponential temperature dependence in low temperature for specific heat and superfluid density. If there are line nodes on the FS, both the specific heat and superfluid density will show power law temperature dependence. While for super-conducting state with finite "Fermi Arc", the low temperature behavior of specific heat appears like there are some "residue density of states" on the Fermi level. Currently there are some experimental evidence indicating the existence of low

energy quasi-particles in the super-conducting phase[15, 31, 32]. But we still need further experimental data to make the conclusion.

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